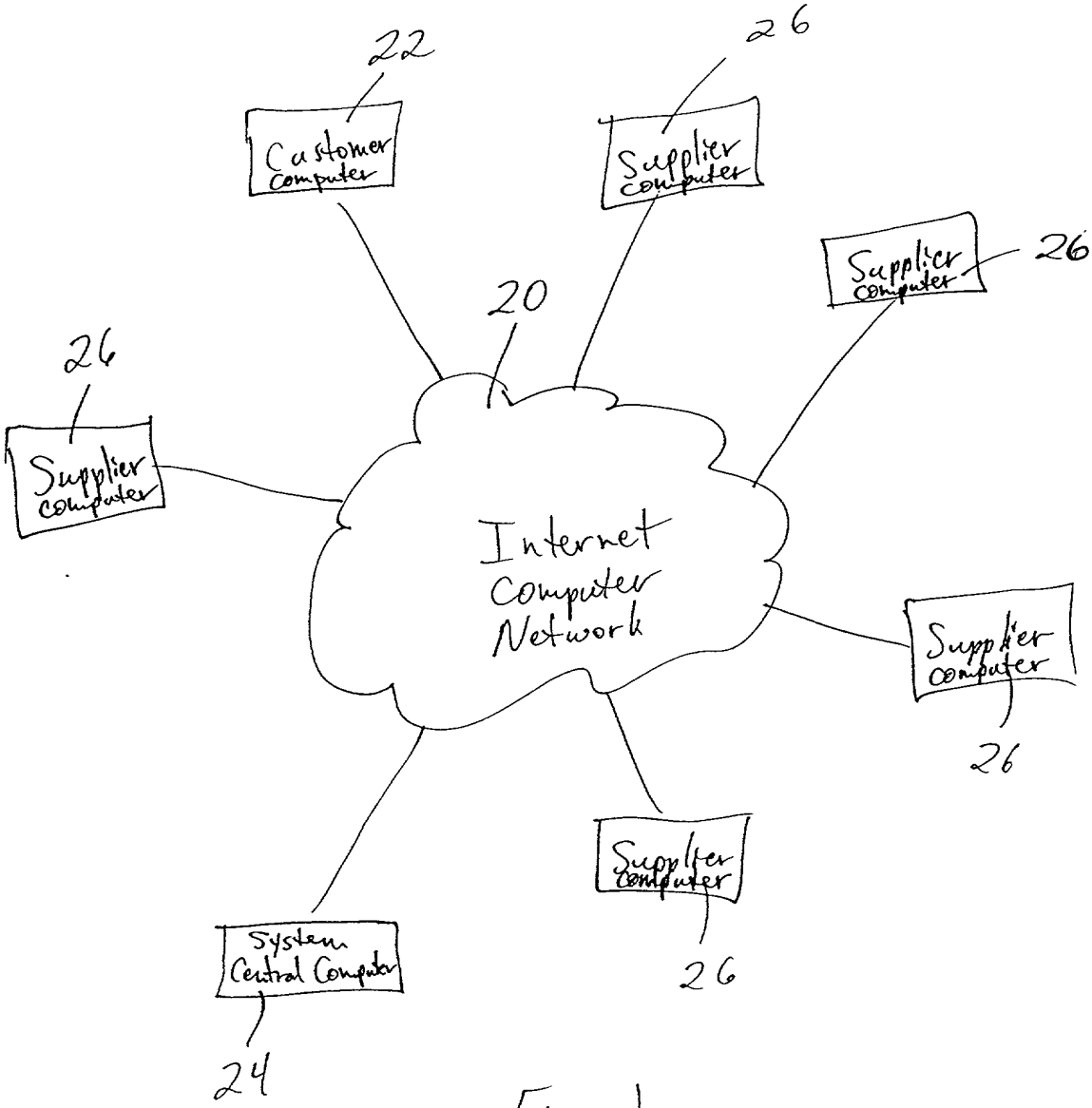

22
Customer computer
26
Supplier computer
Supplier computer
26
20
26
Supplier computer
Internet Computer Network
Supplier computer
26
Supplier computer
26
System Central Computer
24

Fig. 1

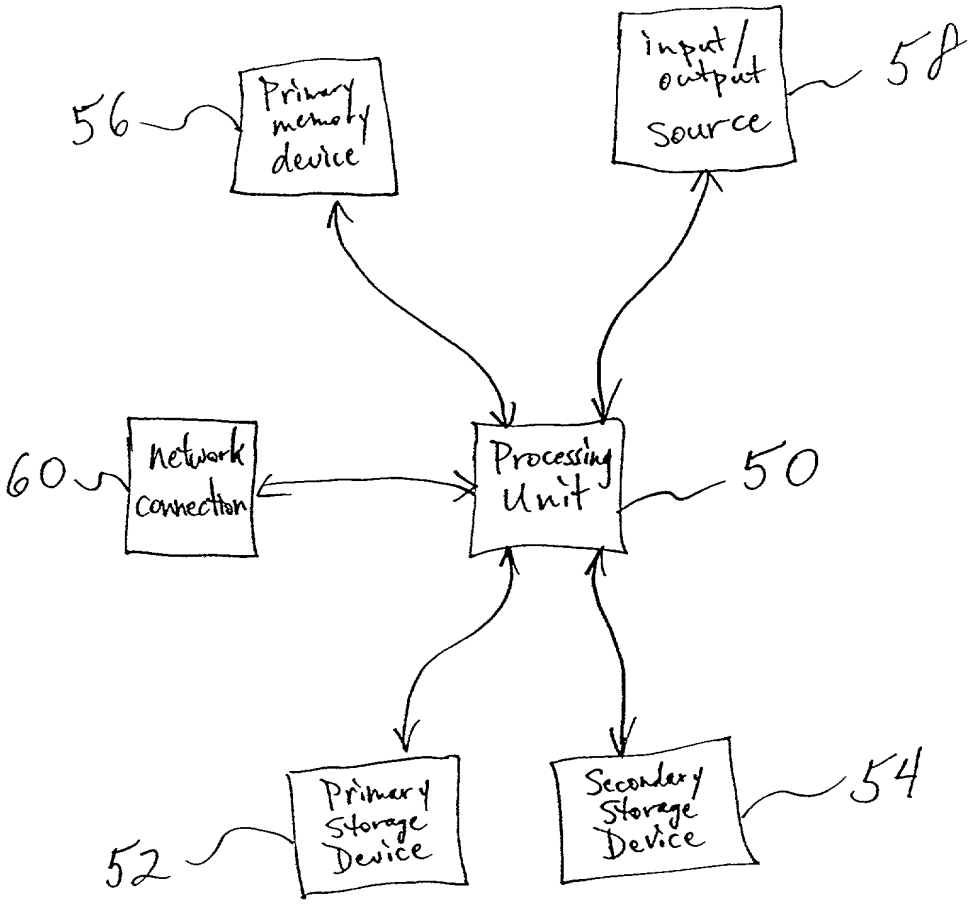

56
Primary memory device
input/output source
58
60
network connection
Processing Unit
50
52
Primary Storage Device
Secondary Storage Device
54

Fig. 2

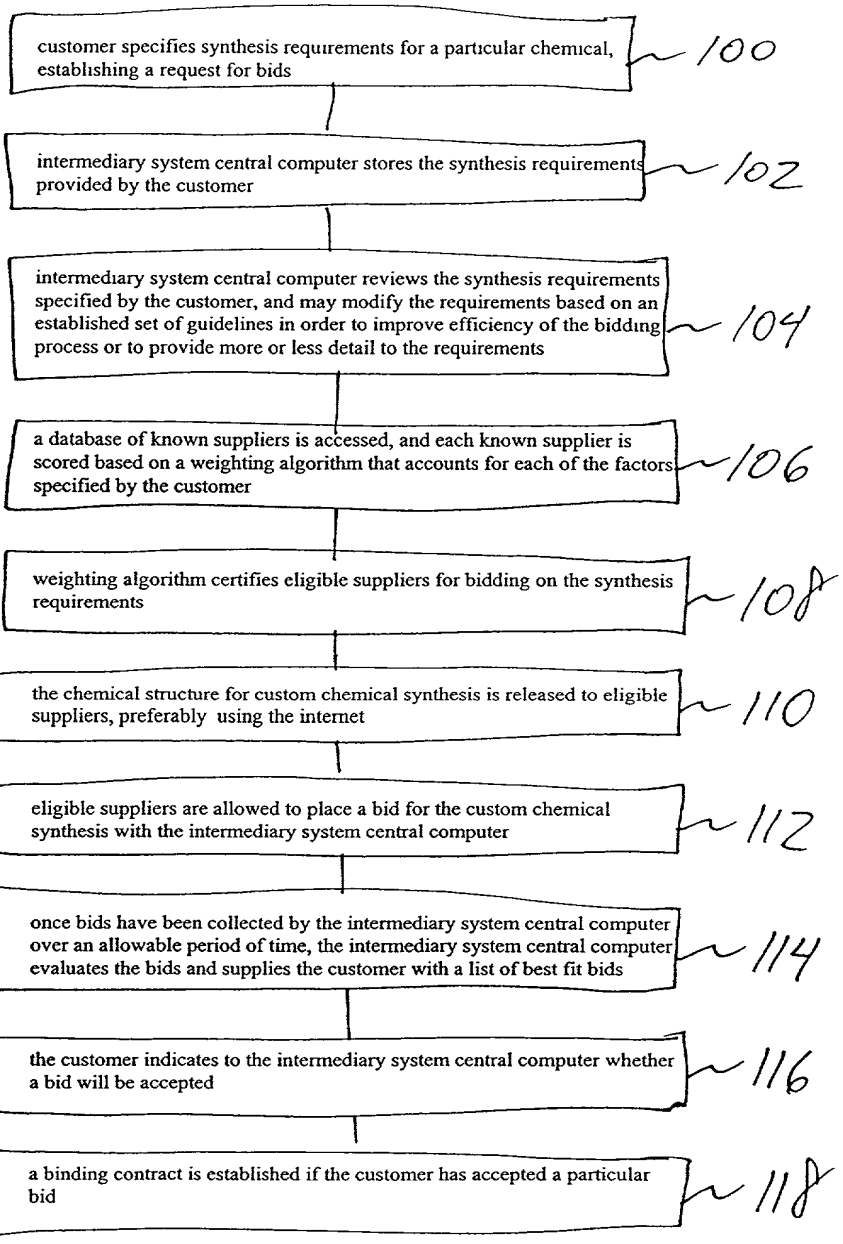

customer specifies synthesis requirements for a particular chemical, establishing a request for bids
100
intermediary system central computer stores the synthesis requirements provided by the customer
102
intermediary system central computer reviews the synthesis requirements specified by the customer, and may modify the requirements based on an established set of guidelines in order to improve efficiency of the bidding process or to provide more or less detail to the requirements
104
a database of known suppliers is accessed, and each known supplier is scored based on a weighting algorithm that accounts for each of the factors specified by the customer
106
weighting algorithm certifies eligible suppliers for bidding on the synthesis requirements
108
the chemical structure for custom chemical synthesis is released to eligible suppliers, preferably using the internet
110
eligible suppliers are allowed to place a bid for the custom chemical synthesis with the intermediary system central computer
112
once bids have been collected by the intermediary system central computer over an allowable period of time, the intermediary system central computer evaluates the bids and supplies the customer with a list of best fit bids
114
the customer indicates to the intermediary system central computer whether a bid will be accepted
116
a binding contract is established if the customer has accepted a particular bid
118

Fig. 3

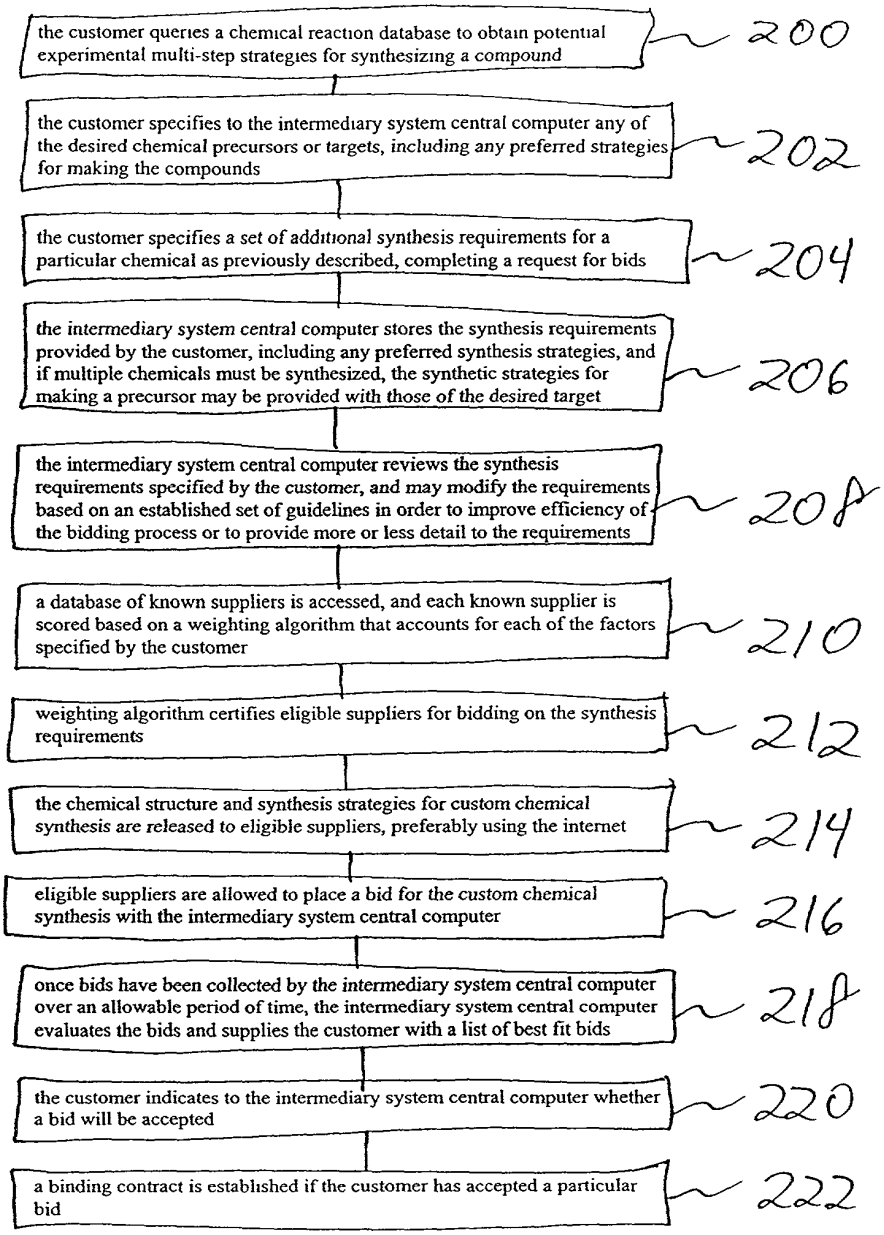

the customer queries a chemical reaction database to obtain potential experimental multi-step strategies for synthesizing a compound
200
the customer specifies to the intermediary system central computer any of the desired chemical precursors or targets, including any preferred strategies for making the compounds
202
the customer specifies a set of additional synthesis requirements for a particular chemical as previously described, completing a request for bids
204
the intermediary system central computer stores the synthesis requirements provided by the customer, including any preferred synthesis strategies, and if multiple chemicals must be synthesized, the synthetic strategies for making a precursor may be provided with those of the desired target
206
the intermediary system central computer reviews the synthesis requirements specified by the customer, and may modify the requirements based on an established set of guidelines in order to improve efficiency of the bidding process or to provide more or less detail to the requirements
208
a database of known suppliers is accessed, and each known supplier is scored based on a weighting algorithm that accounts for each of the factors specified by the customer
210
weighting algorithm certifies eligible suppliers for bidding on the synthesis requirements
212
the chemical structure and synthesis strategies for custom chemical synthesis are released to eligible suppliers, preferably using the internet
214
eligible suppliers are allowed to place a bid for the custom chemical synthesis with the intermediary system central computer
216
once bids have been collected by the intermediary system central computer over an allowable period of time, the intermediary system central computer evaluates the bids and supplies the customer with a list of best fit bids
218
the customer indicates to the intermediary system central computer whether a bid will be accepted
220
a binding contract is established if the customer has accepted a particular bid
222

Fig. 4

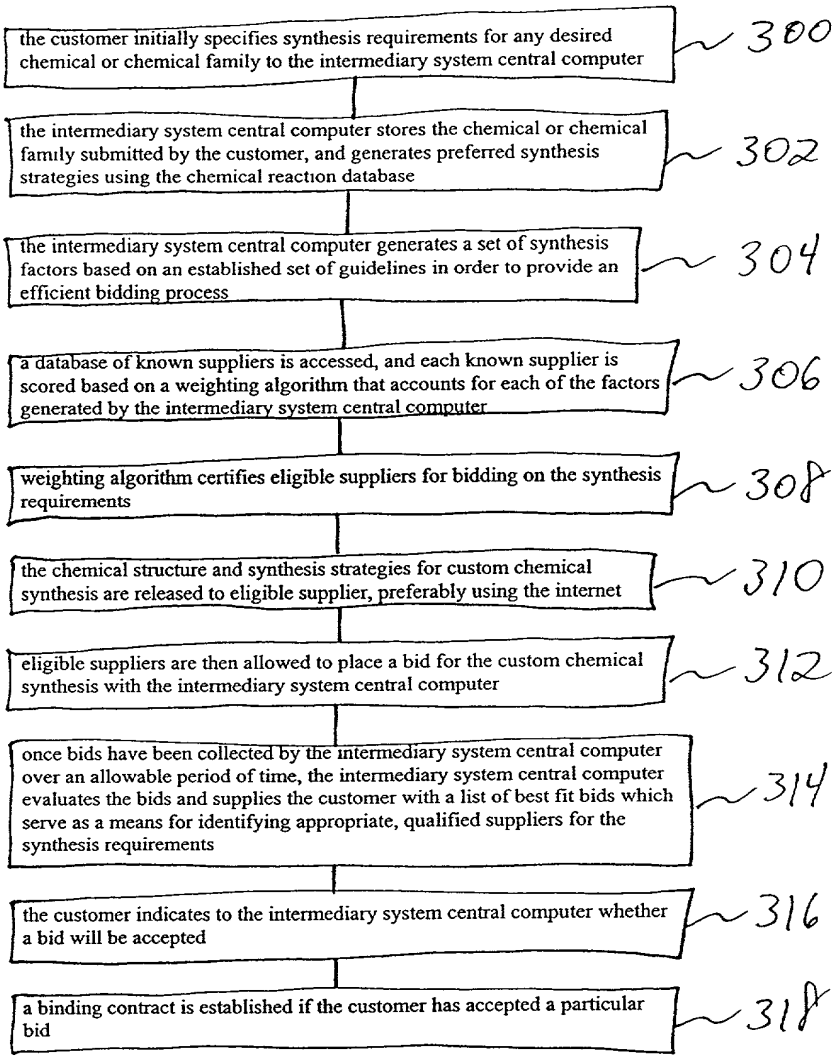

the customer initially specifies synthesis requirements for any desired chemical or chemical family to the intermediary system central computer
300
the intermediary system central computer stores the chemical or chemical family submitted by the customer, and generates preferred synthesis strategies using the chemical reaction database
302
the intermediary system central computer generates a set of synthesis factors based on an established set of guidelines in order to provide an efficient bidding process
304
a database of known suppliers is accessed, and each known supplier is scored based on a weighting algorithm that accounts for each of the factors generated by the intermediary system central computer
306
weighting algorithm certifies eligible suppliers for bidding on the synthesis requirements
308
the chemical structure and synthesis strategies for custom chemical synthesis are released to eligible supplier, preferably using the internet
310
eligible suppliers are then allowed to place a bid for the custom chemical synthesis with the intermediary system central computer
312
once bids have been collected by the intermediary system central computer over an allowable period of time, the intermediary system central computer evaluates the bids and supplies the customer with a list of best fit bids which serve as a means for identifying appropriate, qualified suppliers for the synthesis requirements
314
the customer indicates to the intermediary system central computer whether a bid will be accepted
316
a binding contract is established if the customer has accepted a particular bid
318

Fig. 5

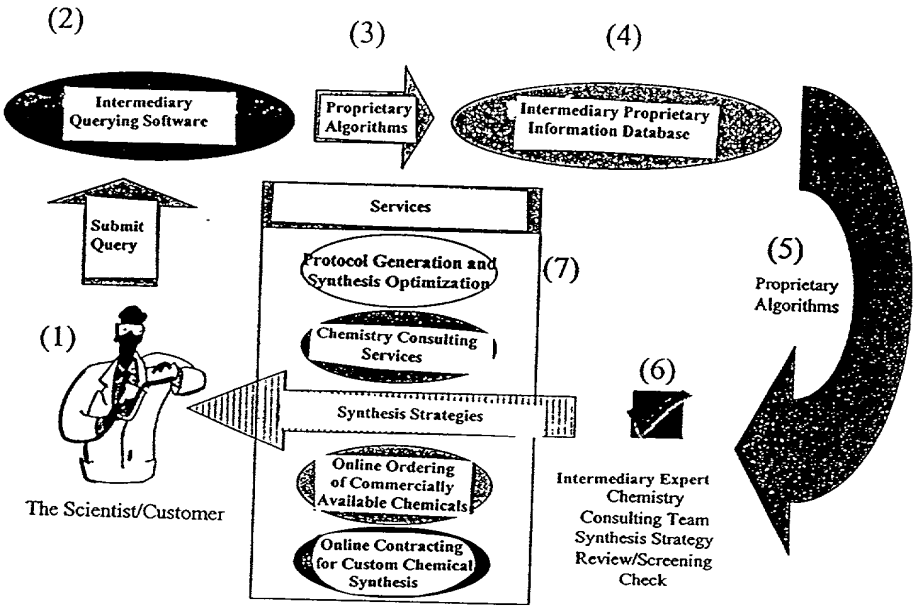
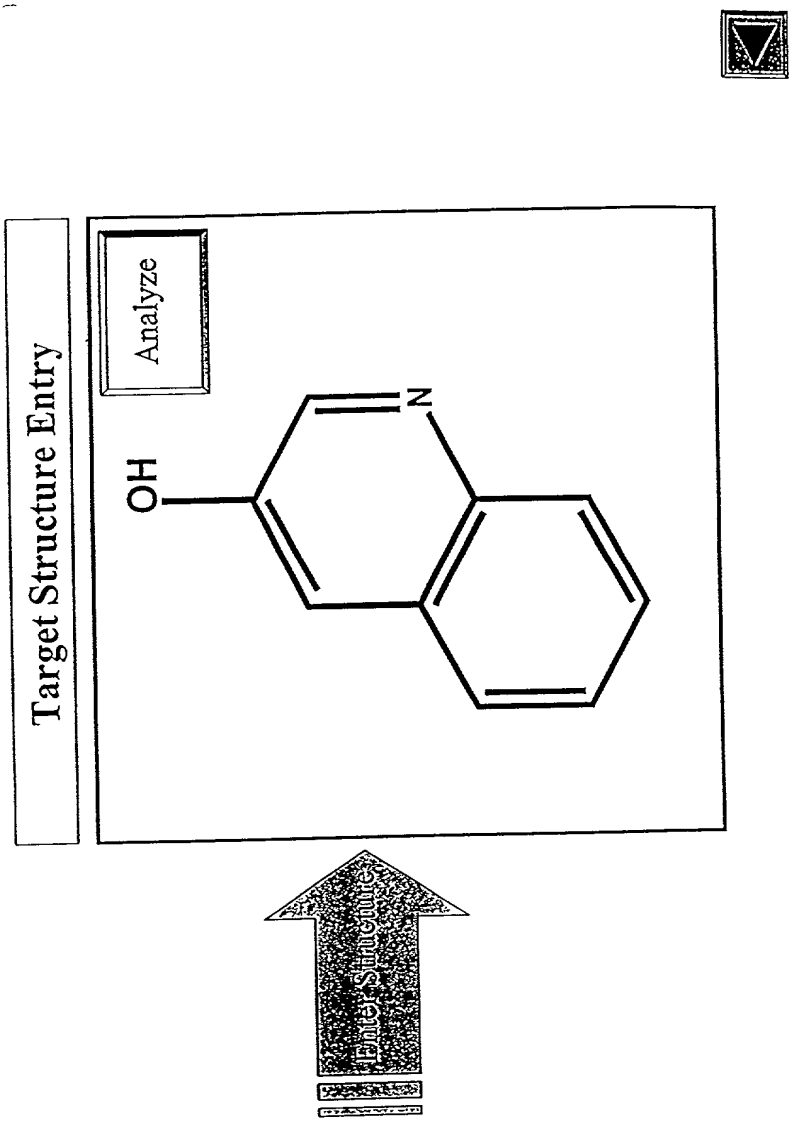

(2)
(3)
(4)
Intermediary Querying Software
Proprietary Algorithms
Intermediary Proprietary Information Database
Submit Query
Services
Protocol Generation and Synthesis Optimization
(7)
(5)
Proprietary Algorithms
(1)
Chemistry Consulting Services
(6)
Synthesis Strategies
Online Ordering of Commercially Available Chemicals
Online Contracting for Custom Chemical Synthesis
The Scientist/Customer
Intermediary Expert Chemistry Consulting Team Synthesis Strategy Review/Screening Check

Fig. 6



400

Fig. 7

Fig 8

420

Synthesis Strategies

Routes	Yield %	# of steps to ACD	# of Purification Steps Required	Cost Per mg of product	Add Synthetic Routes to Project
Route 1	86	6	4	$2,000	X
Route 2	75	N/A	N/A	N/A	X
Route 3	**71**	**4**	**3**	**$6,434**	X
Route 4	63	5	2	$200	X
Route 5	44	10	8	$22,050	
Route 6	31	7	6	$15,427	
Route 7	24	5	5	$155	
Route 8	20	6	4	$4,450	
Route 9	17	6	5	$344	
Route 10	9	N/A	N/A	N/A	
Route 11	4	6	6	$36,000	

Route 3:

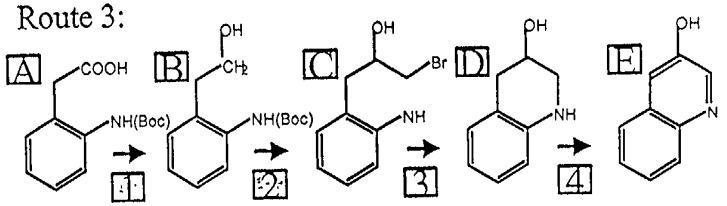
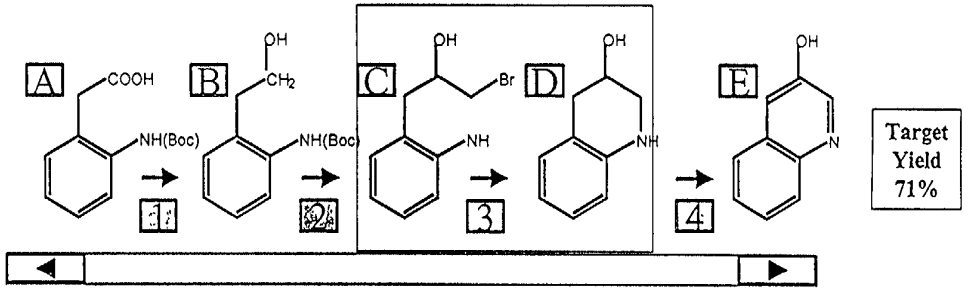


Fig. 9

440

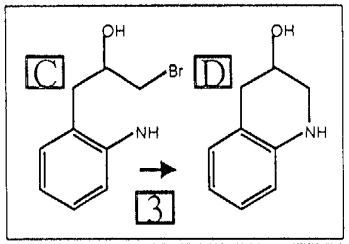
Synthesis Reaction Planner



Amt of Target Compound Desired: XX (g)

Step	Starting Materials	ID #	Quantity Required	Suggested Supplier	Cost	Place Orders to Suppliers	Request Bids	Inventory location/ Expected arrival date	Scheduled date for completion
3	DMF					☑			
	KOH							A10233	
	C						☑		
	YYYY					☑			

Synthesis Protocol Generation



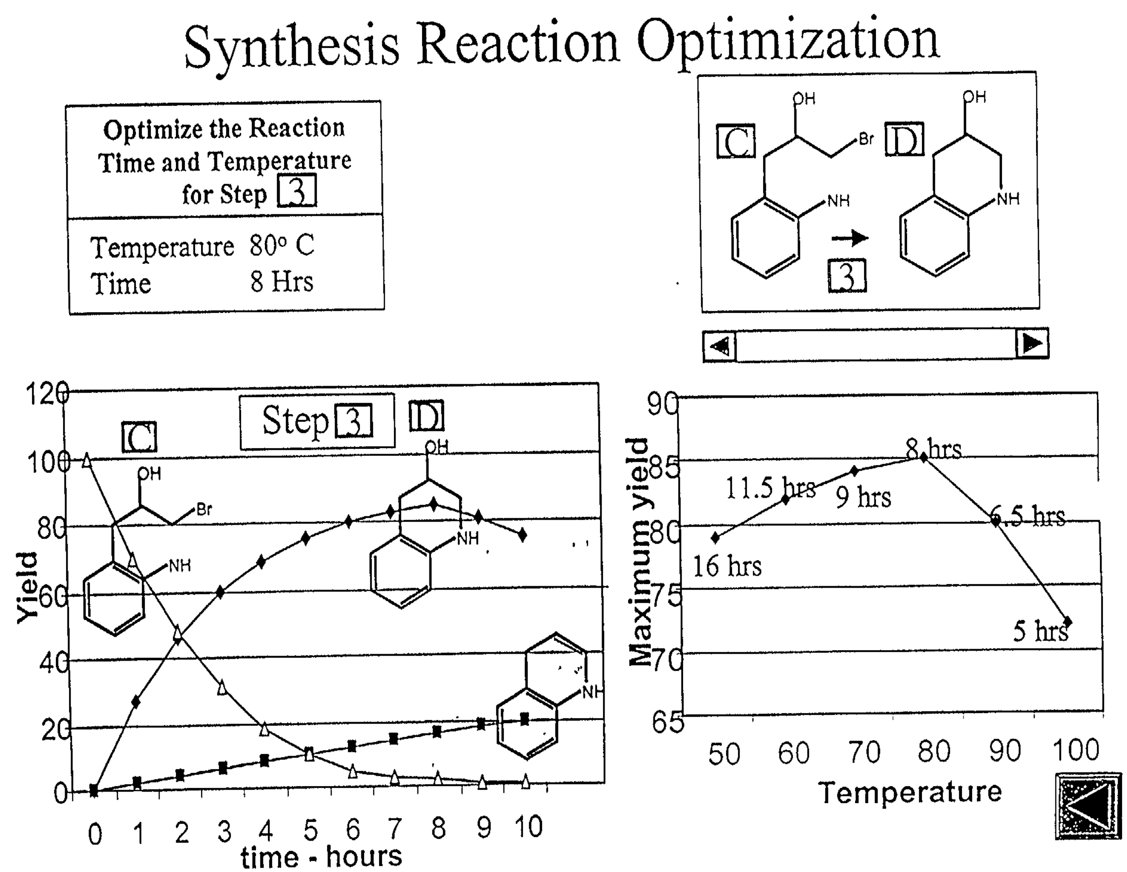
Target Yield 89%

◁ ▷

Step	Starting materials in order of addition	Amount (g)	Inventory ID and Location	Solvent	Amount (ml)	Recommended purification steps	Time	Temp.	Scheduled date for completion
						View Side Products			
3							Optimize		

Fig. 10

410


Synthesis Reaction Optimization
Optimize the Reaction Time and Temperature for Step 3
Temperature 80° C
Time 8 Hrs
C
OH
Br
NH
D
OH
NH
3
Step 3
C
D
Yield
120
100
80
60
40
20
0
0 1 2 3 4 5 6 7 8 9 10
time - hours
Maximum yield
90
85
80
75
70
65
50 60 70 80 90 100
Temperature
16 hrs
11.5 hrs
9 hrs
8 hrs
6.5 hrs
5 hrs

480

Fig. 11

Request Bids

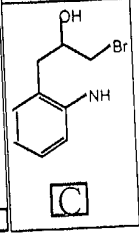
Target	Level of Confidentiality Required	Desired Quantity	Cost	Level of Purity	Stereo-chemical Require-ments	Suggested Strategies	Request Bids
	Ultra High Medium Low None	10 g	< $40,000	⌐99% ⌐95% ⌐90%	None	Edit	Request Preliminary Bids Request Binding Bids

Fig. 12

500